Chaoyu He

List of Publications by Year in descending order

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83 papers	2,151 citations	201674 27 h-index	243625 44 g-index
83 all docs	83 docs citations	83 times ranked	2131 citing authors

#	Article	IF	Citations
1	Notable effect of magnetic order on the phonon transport in semi-hydrogenated graphene. Applied Physics Letters, 2022, 120, .	3.3	8
2	Strain induced magnetic hysteresis in MoS₂ and WS₂ monolayers with symmetric double sulfur vacancy defects. Physical Chemistry Chemical Physics, 2022, 24, 17263-17270.	2.8	1
3	First-principles study on the electronic, mechanical and optical properties for silicon allotropes in hexagonal 2â€“7 stacking orders. Scripta Materialia, 2022, 219, 114843.	5.2	7
4	Potential thermoelectric candidate monolayer silicon diphosphide (SiP2) from a first-principles calculation. Computational Materials Science, 2021, 188, 110154.	3.0	10
5	Robust transport of charge carriers in in-plane 1Tâ€²-2H MoTe2 homojunctions with ohmic contact. Nano Research, 2021, 14, 1311-1318.	10.4	16
6	Two-Dimensional Carbon Allotropes and Nanoribbons based on 2,6-Polyazulene Chains: Stacking Stabilities and Electronic Properties. Journal of Physical Chemistry Letters, 2021, 12, 732-738.	4.6	41
7	Newly discovered graphyne allotrope with rare and robust Dirac node loop. Nanoscale, 2021, 13, 3564-3571.	5.6	33
8	New structure candidates for the experimentally synthesized heptazine-based and triazine-based two dimensional graphitic carbon nitride. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 128, 114535.	2.7	2
9	Bayesian optimization-based design of defect gamma-graphyne nanoribbons with high thermoelectric conversion efficiency. Carbon, 2021, 176, 52-60.	10.3	25
10	Dirac Semimetal Protected by Nonsymmorphic Mirror Symmetries in TPHâ€Graphene. Physica Status Solidi - Rapid Research Letters, 2021, 15, 2100039.	2.4	7
11	Enhanced and spin-dependent infrared optical response of silicene/silicane superlattices with Cr adsorption. Journal Physics D: Applied Physics, 2021, 54, 405106.	2.8	0
12	New Two-Dimensional Wide Band Gap Hydrocarbon Insulator by Hydrogenation of a Biphenylene Sheet. Journal of Physical Chemistry Letters, 2021, 12, 8889-8896.	4.6	26
13	Tunable topologically nontrivial states in newly discovered graphyne allotropes: from Dirac nodal grid to Dirac nodal loop. Nanotechnology, 2021, 32, 485705.	2.6	4
14	SIn₂Te/TeIn₂Se: a type-II heterojunction as a water-splitting photocatalyst with high solar energy harvesting. Journal of Materials Chemistry C, 2021, 9, 7734-7744.	5.5	10
15	Type-II lateral SnSe/GeTe heterostructures for solar photovoltaic applications with high efficiency. Nanoscale Advances, 2021, 3, 3643-3649.	4.6	7
16	The intrinsic thermal transport properties of the biphenylene network and the influence of hydrogenation: a first-principles study. Journal of Materials Chemistry C, 2021, 9, 16945-16951.	5.5	26
17	High-Throughput Screening of Two-Dimensional Planar sp² Carbon Space Associated with a Labeled Quotient Graph. Journal of Physical Chemistry Letters, 2021, 12, 11511-11519.	4.6	34
18	KP15: Natural van der Waals material with ultra-low thermal conductivity and excellent thermoelectric performance. Journal of Applied Physics, 2021, 130, 195104.	2.5	0

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19	Electronic and Spinâ€Dependent Optical Properties of Feâ€Adsorbed Armchair Silicene/Silicane Superlattices. Physica Status Solidi - Rapid Research Letters, 2020, 14, 1900494.	2.4	3
20	Quasi-bonding driven abnormal isotropic thermal transport in intrinsically anisotropic nanostructure: a case of study of a phosphorus nanotube array. Nanotechnology, 2020, 31, 095704.	2.6	3
21	Strain effect on phonon transport in open framework Si24: A first-principles study. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 118, 113870.	2.7	7
22	Photogalvanicâ€Effectâ€Induced Spinâ€Polarized Current in Defective Silicane with H Vacancies. Physica Status Solidi - Rapid Research Letters, 2020, 14, 2000395.	2.4	13
23	Systematic Enumeration of Lowâ€Energy Graphyne Allotropes Based on a Coordinationâ€Constrained Searching Strategy. Physica Status Solidi - Rapid Research Letters, 2020, 14, 2000437.	2.4	17
24	Geometries and Electronic Properties of Black Phosphorus/MoS2 Heterostructure with P Atom Vacancies: First Principles Calculations. Journal of Electronic Materials, 2020, 49, 5730-5738.	2.2	2
25	Optoelectronic properties of type-II SePtTe/InS van der Waals heterojunction. Journal of Applied Physics, 2020, 128, .	2.5	12
26	Excellent thermoelectric performance of open framework Si24 nanowires from density functional based tight-binding calculation. Journal of Applied Physics, 2020, 128, 215108.	2.5	1
27	Band offsets engineering in asymmetric Janus bilayer transition-metal dichalcogenides. Journal of Physics Condensed Matter, 2020, 32, 035502.	1.8	6
28	Tunable photoelectronic properties of hydrogenated-silicene/halogenated-silicene superlattices for water splitting. Journal of Applied Physics, 2020, 127, .	2.5	18
29	Intrinsic piezoelectricity of monolayer group IVâ€“V MX2: SiP2, SiAs2, GeP2, and GeAs2. Applied Physics Letters, 2020, 116, .	3.3	30
30	Few-Layer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mi>Î²</mml:mi></mml:math> - <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mrow><mml:mi>Sn</mml:mi><mml:mi>Se</mml:mi></mml:mrow></mml:math> with Strong Visible Light Absorbance and Ultrahigh Carrier Mobility. Physical Review Applied, 2020, 13, .	3.8	8
31	Theoretical prediction of low-energy Stone-Wales graphene with an intrinsic type-III Dirac cone. Physical Review B, 2020, 101, .	3.2	53
32	Ferromagnetism triggered by nitrogen defects in graphitic carbon nitride. Journal Physics D: Applied Physics, 2020, 53, 495002.	2.8	2
33	Lowâ€Energy GeP Monolayers with Natural Typeâ€II Homojunctions for SunLightâ€Driven Water Splitting. Physica Status Solidi - Rapid Research Letters, 2019, 13, 1900470.	2.4	12
34	Si-Cmma: A silicon thin film with excellent stability and Dirac nodal loop. Physical Review B, 2019, 100, .	3.2	36
35	Ge3P2: New viable two-dimensional semiconductors with ultrahigh carrier mobility. Applied Surface Science, 2019, 497, 143803.	6.1	17
36	Stone-Wales graphene: A two-dimensional carbon semimetal with magic stability. Physical Review B, 2019, 99, .	3.2	95

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37	Strain effects on magnetic states of monolayer MoS2 doped with group IIIA to VA atoms. Physica E: Low-Dimensional Systems and Nanostructures, 2019, 114, 113609.	2.7	8
38	First-principles prediction of a new ground state for surface-oxidized phosphorene with remarkable piezoelectricity. Journal Physics D: Applied Physics, 2019, 52, 295301.	2.8	1
39	First-principles prediction of three new graphitic C3N4 allotropes with potentials for application in sun-light-driven water splitting. Physica B: Condensed Matter, 2019, 562, 131-134.	2.7	12
40	The thermoelectric properties of monolayer SiP and GeP from first-principles calculations. Journal of Applied Physics, 2019, 126, .	2.5	14
41	First-principles prediction of two atomic-thin phosphorene allotropes with potentials for sun-light-driven water splitting. Journal of Physics Condensed Matter, 2019, 31, 075702.	1.8	7
42	Strain engineering the structures and electronic properties of Janus monolayer transition-metal dichalcogenides. Journal of Applied Physics, 2019, 125, .	2.5	39
43	Allotropes of Phosphorus with Remarkable Stability and Intrinsic Piezoelectricity. Physical Review Applied, 2018, 9, .	3.8	16
44	Stochastic generation of complex crystal structures combining group and graph theory with application to carbon. Physical Review B, 2018, 97, .	3.2	114
45	Surface oxidation: an effective way to induce piezoelectricity in 2D black phosphorus. Journal Physics D: Applied Physics, 2018, 51, 12LT01.	2.8	11
46	First-principles study of magnetic properties of ultra-thin MoSi2 films. Journal of Applied Physics, 2018, 123, 104304.	2.5	5
47	Thermal and thermoelectric properties of monolayer indium triphosphide (InP₃): a first-principles study. Journal of Materials Chemistry A, 2018, 6, 21532-21541.	10.3	91
48	The thermoelectric performance of dumbbell silicene nanoribbons. Fullerenes Nanotubes and Carbon Nanostructures, 2018, 26, 511-517.	2.1	1
49	Thermoelectric properties of four typical silicon allotropes. Modelling and Simulation in Materials Science and Engineering, 2018, 26, 085006.	2.0	7
50	Complex Low Energy Tetrahedral Polymorphs of Group IV Elements from First Principles. Physical Review Letters, 2018, 121, 175701.	7.8	95
51	First-principles prediction of two hexagonal silicon crystals as potential absorbing layer materials for solar-cell application. Journal of Applied Physics, 2018, 124, .	2.5	10
52	A novel WS₂/NbSe₂ vdW heterostructure as an ultrafast charging and discharging anode material for lithium-ion batteries. Journal of Materials Chemistry A, 2018, 6, 17040-17048.	10.3	53
53	Doping Induced Abnormal Contraction and Significant Reduction of Lattice Thermal Conductivity of Open Framework Si24. ES Energy & Environments, 2018, , .	1.1	7
54	Ab initioprediction of a new allotrope of two-dimensional silicon. Physica Status Solidi - Rapid Research Letters, 2017, 11, 1600422.	2.4	9

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55	Five low energy phosphorene allotropes constructed through gene segments recombination. Scientific Reports, 2017, 7, 46431.	3.3	31
56	First-principles study of the structures and fundamental electronic properties of two-dimensional P_{0.5}As_{0.5}alloy. Physica Status Solidi (B): Basic Research, 2017, 254, 1700157.	1.5	6
57	Lattice thermal conductivity of borophene from first principle calculation. Scientific Reports, 2017, 7, 45986.	3.3	60
58	Optimizing the thermoelectric performance of graphyne nanotube via applying radial strain. Journal of Applied Physics, 2017, 121, 125112.	2.5	5
59	Effect of hydrogen passivation on the decoupling of graphene on SiC(0001) substrate: First-principles calculations. Scientific Reports, 2017, 7, 8461.	3.3	4
60	Potential thermoelectric material open framework Si24 from a first-principles study. Journal Physics D: Applied Physics, 2017, 50, 425501.	2.8	15
61	New candidate for the simple cubic carbon sample shock-synthesized by compression of the mixture of carbon black and tetracyanoethylene. Carbon, 2017, 112, 91-96.	10.3	27
62	Firstâ€principles prediction of a novel hexagonal phosphorene allotrope. Physica Status Solidi - Rapid Research Letters, 2016, 10, 563-565.	2.4	28
63	Charge transport properties of graphene: Effects of Cu-based gate electrode. Journal of Applied Physics, 2016, 120, .	2.5	1
64	Direct and quasi-direct band gap silicon allotropes with remarkable stability. Physical Chemistry Chemical Physics, 2016, 18, 9682-9686.	2.8	49
65	Two-dimensional topological insulators with tunable band gaps: Single-layer HgTe and HgSe. Scientific Reports, 2015, 5, 14115.	3.3	50
66	Stability of two-dimensional PN monolayer sheets and their electronic properties. Physical Chemistry Chemical Physics, 2015, 17, 32009-32015.	2.8	47
67	M585, a low energy superhard monoclinic carbon phase. Solid State Communications, 2014, 181, 24-27.	1.9	25
68	Effective Fermi level tuning of Bi2Se3 by introducing CdBi/CaBi dopant. RSC Advances, 2014, 4, 10499.	3.6	1
69	The structural, electronic and magnetic properties of bi-layered MoS2 with transition-metals doped in the interlayer. RSC Advances, 2013, 3, 12939.	3.6	33
70	Density functional theory study of Fe adatoms adsorbed monolayer and bilayer MoS2 sheets. Journal of Applied Physics, 2013, 114, .	2.5	35
71	Structures, stability, mechanical and electronic properties of Î±-boron andÎ±*-boron. AIP Advances, 2013, 3, .	1.3	18
72	Two viable three-dimensional carbon semiconductors with an entirely sp²configuration. Physical Chemistry Chemical Physics, 2013, 15, 680-684.	2.8	48

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73	Low energy three-dimensional hydrocarbon crystal from cold compression of benzene. Journal of Physics Condensed Matter, 2013, 25, 205403.	1.8	10
74	Modulation effect of hydrogen and fluorine decoration on the surface work function of BN sheets. AIP Advances, 2012, 2, .	1.3	18
75	Magnetic Properties of Single Transition-Metal Atom Absorbed Graphdiyne and Graphyne Sheet from DFT+U Calculations. Journal of Physical Chemistry C, 2012, 116, 26313-26321.	3.1	264
76	Effects of contact oxidization on the transport properties of Au/ZGNR junctions. Physica Status Solidi - Rapid Research Letters, 2012, 6, 457-459.	2.4	4
77	Structures, stability and electronic properties of two- or four-segment BN/C nanotubes. , 2012, , .		0
78	New superhard carbon phases between graphite and diamond. Solid State Communications, 2012, 152, 1560-1563.	1.9	89
79	Structure, stability and electronic properties of tricycle type graphane. Physica Status Solidi - Rapid Research Letters, 2012, 6, 427-429.	2.4	43
80	Four superhard carbon allotropes: a first-principles study. Physical Chemistry Chemical Physics, 2012, 14, 8410.	2.8	66
81	Z-BN: a novel superhard boron nitride phase. Physical Chemistry Chemical Physics, 2012, 14, 10967.	2.8	72
82	Hydrogenated graphene: Structures and surface work function. , 2012, , .		2
83	Transport Properties of Zigzag Graphene Nanoribbons Decorated by Carboxyl Group Chains. Journal of Physical Chemistry C, 2011, 115, 21893-21898.	3.1	8